

Study guide: Time-dependent problems and variational forms

Hans Petter Langtangen^{1,2}

Center for Biomedical Computing, Simula Research Laboratory¹

Department of Informatics, University of Oslo²

Oct 30, 2015

Time-dependent problems

- So far: used the finite element framework for discretizing in space
- What about $u_t = u_{xx} + f$?
 - 1 Use finite differences in time to obtain a set of recursive spatial problems
 - 2 Solve the spatial problems by the finite element method

Example: diffusion problem

$$\begin{aligned} \frac{\partial u}{\partial t} &= \alpha \nabla^2 u + f(\mathbf{x}, t), & \mathbf{x} \in \Omega, t \in (0, T] \\ u(\mathbf{x}, 0) &= I(\mathbf{x}), & \mathbf{x} \in \Omega \\ \frac{\partial u}{\partial n} &= 0, & \mathbf{x} \in \partial\Omega, t \in (0, T] \end{aligned}$$

A Forward Euler scheme: ideas

$$[D_t^+ u = \alpha \nabla^2 u + f]^n, \quad n = 1, 2, \dots, N_t - 1$$

Solving wrt u^{n+1} :

$$u^{n+1} = u^n + \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))$$

- $u^n = \sum_j c_j^n \psi_j \in V$, $u^{n+1} = \sum_j c_j^{n+1} \psi_j \in V$
- Compute u^0 from I
- Compute u^{n+1} from u^n by solving the PDE for u^{n+1} at each time level

A Forward Euler scheme: stages in the discretization

- $u_e(\mathbf{x}, t)$: exact solution of the PDE problem
- $u_e^n(\mathbf{x})$: exact solution of time-discrete problem (after applying a finite difference scheme in time)
- $u_e^n(\mathbf{x}) \approx u^n = \sum_{j \in \mathcal{I}_h} c_j^n \psi_j$ = solution of the time- and space-discrete problem (after applying a Galerkin method in space)

$$\frac{\partial u_e}{\partial t} = \alpha \nabla^2 u_e + f(\mathbf{x}, t)$$

$$u_e^{n+1} = u_e^n + \Delta t (\alpha \nabla^2 u_e^n + f(\mathbf{x}, t_n))$$

$$u_e^n \approx u^n = \sum_{j=0}^N c_j^n \psi_j(\mathbf{x}), \quad u_e^{n+1} \approx u^{n+1} = \sum_{j=0}^N c_j^{n+1} \psi_j(\mathbf{x})$$

$$R = u^{n+1} - u^n - \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))$$

A Forward Euler scheme: weighted residual (or Galerkin) principle

$$R = u^{n+1} - u^n - \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))$$

The weighted residual principle:

$$\int_{\Omega} R w \, dx = 0, \quad \forall w \in W$$

results in

$$\int_{\Omega} [u^{n+1} - u^n - \Delta t (\alpha \nabla^2 u^n + f(\mathbf{x}, t_n))] w \, dx = 0, \quad \forall w \in W$$

Galerkin: $W = V$, $w = v$

A Forward Euler scheme: integration by parts

Isolating the unknown u^{n+1} on the left-hand side:

$$\int_{\Omega} u^{n+1} \psi_i dx = \int_{\Omega} [u^n + \Delta t (\alpha \nabla^2 u^n + f(x, t_n))] \psi_i dx$$

Integration by parts of $\int \alpha (\nabla^2 u^n) \psi_i dx$:

$$\int_{\Omega} \alpha (\nabla^2 u^n) \psi_i dx = - \int_{\Omega} \alpha \nabla u^n \cdot \nabla \psi_i dx + \underbrace{\int_{\partial \Omega} \alpha \frac{\partial u^n}{\partial n} \psi_i dx}_{=0 \quad \leftarrow \quad \partial u^n / \partial n = 0}$$

Variational form:

$$\int_{\Omega} u^{n+1} \psi_i dx = \int_{\Omega} u^n \psi_i dx - \Delta t \int_{\Omega} \alpha \nabla u^n \cdot \nabla \psi_i dx + \Delta t \int_{\Omega} f^n \psi_i dx, \quad \forall \psi_i \in V$$

New notation for the solution at the most recent time levels

- u and u : the spatial unknown function to be computed
- u_1 and u_{-1} : the spatial function at the previous time level $t - \Delta t$
- u_2 and u_{-2} : the spatial function at $t - 2\Delta t$
- This new notation gives close correspondence between code and math

$$\int_{\Omega} uv dx = \int_{\Omega} u_1 v dx - \Delta t \int_{\Omega} \alpha \nabla u_1 \cdot \nabla v dx + \Delta t \int_{\Omega} f^n v dx$$

or shorter

$$(u, v) = (u_1, v) - \Delta t (\alpha \nabla u_1, \nabla v) + \Delta t (f^n, v)$$

Deriving the linear systems

- $u = \sum_{j=0}^N c_j \psi_j(x)$
- $u_1 = \sum_{j=0}^N c_{1,j} \psi_j(x)$
- $\forall v \in V$: for $v = \psi_i$, $i = 0, \dots, N$

Insert these in

$$(u, \psi_i) = (u_1, \psi_i) - \Delta t (\alpha \nabla u_1, \nabla \psi_i) + \Delta t (f^n, \psi_i)$$

and order terms as matrix-vector products ($i = 0, \dots, N$):

$$\sum_{j=0}^N \underbrace{(\psi_i, \psi_j)}_{M_{i,j}} c_j = \sum_{j=0}^N \underbrace{(\psi_i, \psi_j)}_{M_{i,j}} c_{1,j} - \Delta t \sum_{j=0}^N \underbrace{(\nabla \psi_i, \alpha \nabla \psi_j)}_{K_{i,j}} c_{1,j} + \Delta t (f^n, \psi_i)$$

Structure of the linear systems

$$Mc = Mc_1 - \Delta t Kc_1 + \Delta t f$$

$$\begin{aligned} M &= \{M_{i,j}\}, \quad M_{i,j} = (\psi_i, \psi_j), \quad i, j \in \mathcal{I}_s \\ K &= \{K_{i,j}\}, \quad K_{i,j} = (\nabla \psi_i, \alpha \nabla \psi_j), \quad i, j \in \mathcal{I}_s \\ f &= \{(f(x, t_n), \psi_i)\}_{i \in \mathcal{I}_s} \\ c &= \{c_i\}_{i \in \mathcal{I}_s} \\ c_1 &= \{c_{1,i}\}_{i \in \mathcal{I}_s} \end{aligned}$$

Computational algorithm

- 1 Compute M and K .
- 2 Initialize u^0 by either interpolation or projection
- 3 For $n = 1, 2, \dots, N_t$:
 - 1 compute $b = Mc_1 - \Delta t Kc_1 + \Delta t f$
 - 2 solve $Mc = b$
 - 3 set $c_1 = c$

Initial condition:

- Either interpolation: $c_{1,j} = I(x_j)$ (finite elements)
- Or projection: solve $\sum_j M_{i,j} c_{1,j} = (I, \psi_i)$, $i \in \mathcal{I}_s$

Example using sinusoidal basis functions

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L), \quad t \in (0, T], \quad (1)$$

$$u(x, 0) = A \cos(\pi x/L) + B \cos(10\pi x/L), \quad x \in [0, L], \quad (2)$$

$$\frac{\partial u}{\partial x} = 0, \quad x = 0, L, \quad t \in (0, T]. \quad (3)$$

$$\psi_i = \cos(i\pi x/L).$$

Approximating the initial condition

$I(x) \in V$ implies perfect approximation of the initial condition:

$$c_{1,1} = A, \quad c_{1,10} = B,$$

while $c_{1,i} = 0$ for $i \neq 1, 10$.

Computing the M and K matrices

Note that ψ_i and ψ_j' are orthogonal on $[0, L]$ such that we only need to compute the diagonal elements $M_{i,i}$ and $K_{i,i}$!

$$M_{0,0} = L, \quad M_{i,i} = L/2, \quad i > 0, \quad K_{0,0} = 0, \quad K_{i,i} = \frac{\pi^2 i^2}{2L}, \quad i > 0.$$

Solving the equation system

$$Lc_0 = Lc_{1,0} - \Delta t \cdot 0 \cdot c_{1,0},$$

$$\frac{L}{2}c_i = \frac{L}{2}c_{1,i} - \Delta t \frac{\pi^2 i^2}{2L}c_{1,i}, \quad i > 0.$$

$$c_i = (1 - \Delta t (\frac{\pi i}{L})^2) c_{1,i}.$$

We actually get a closed-form discrete solution:

$$u_i^n = A(1 - \Delta t (\frac{\pi}{L})^2)^n \cos(\pi x/L) + B(1 - \Delta t (\frac{10\pi}{L})^2)^n \cos(10\pi x/L).$$

Comparing P1 elements with the finite difference method: ideas

- P1 elements in 1D
- Uniform mesh on $[0, L]$ with cell length h
- No Dirichlet conditions: $\psi_i = \varphi_i$, $i = 0, \dots, N = N_n - 1$
- Have found formulas for M and K at the element level
- Have assembled the global matrices
- Have developed corresponding finite difference operator formulas
- M : $h[D_t^+(u + \frac{1}{6}h^2 D_x D_x u)]_i^n$
- K : $h[\alpha D_x D_x u]_i^n$

Comparing P1 elements with the finite difference method: results

Diffusion equation with finite elements is equivalent to

$$[D_t^+(u + \frac{1}{6}h^2 D_x D_x u) = \alpha D_x D_x u + f]_i^n$$

Can lump the mass matrix by Trapezoidal integration and get the standard finite difference scheme

$$[D_t^+ u = \alpha D_x D_x u + f]_i^n$$

Discretization in time by a Backward Euler scheme

Backward Euler scheme in time:

$$[D_t^- u = \alpha \nabla^2 u + f(x, t)]^n$$

$$u_e^n - \Delta t (\alpha \nabla^2 u_e^n + f(x, t_n)) = u_e^{n-1}$$

$$u_e^n \approx u^n = \sum_{j=0}^N c_j^n \psi_j(x), \quad u_e^{n+1} \approx u^{n+1} = \sum_{j=0}^N c_j^{n+1} \psi_j(x)$$

The variational form of the time-discrete problem

$$\int_{\Omega} (u^n \mathbf{v} + \Delta t \alpha \nabla u^n \cdot \nabla \mathbf{v}) \, dx = \int_{\Omega} u^{n-1} \mathbf{v} \, dx + \Delta t \int_{\Omega} f^n \mathbf{v} \, dx, \quad \forall \mathbf{v} \in V$$

or

$$(u, \mathbf{v}) + \Delta t (\alpha \nabla u, \nabla \mathbf{v}) = (u_1, \mathbf{v}) + \Delta t (f^n, \psi_i)$$

The linear system: insert $u = \sum_j c_j \psi_j$ and $u_1 = \sum_j c_{1,j} \psi_j$,

$$(M + \Delta t K) \mathbf{c} = M \mathbf{c}_1 + \Delta t \mathbf{f}$$

Calculations with P1 elements in 1D

Can interpret the resulting equation system as

$$[D_t^-(u + \frac{1}{6} h^2 D_x D_x u) = \alpha D_x D_x u + f]_i^n$$

Lumped mass matrix (by Trapezoidal integration) gives a standard finite difference method:

$$[D_t^- u = \alpha D_x D_x u + f]_i^n$$

Dirichlet boundary conditions

Dirichlet condition at $x = 0$ and Neumann condition at $x = L$:

$$\begin{aligned} u(\mathbf{x}, t) &= u_0(\mathbf{x}, t), & \mathbf{x} \in \partial\Omega_D \\ -\alpha \frac{\partial}{\partial n} u(\mathbf{x}, t) &= g(\mathbf{x}, t), & \mathbf{x} \in \partial\Omega_N \end{aligned}$$

Forward Euler in time, Galerkin's method, and integration by parts:

$$\int_{\Omega} u^{n+1} \mathbf{v} \, dx = \int_{\Omega} (u^n - \Delta t \alpha \nabla u^n \cdot \nabla \mathbf{v}) \, dx + \Delta t \int_{\Omega} f \mathbf{v} \, dx - \Delta t \int_{\partial\Omega_N} g \mathbf{v} \, ds,$$

Requirement: $\mathbf{v} = 0$ on $\partial\Omega_D$

Boundary function

$$u^n(\mathbf{x}) = u_0(\mathbf{x}, t_n) + \sum_{j \in \mathcal{I}_s} c_j^n \psi_j(\mathbf{x})$$

$$\begin{aligned} \sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} \psi_i \psi_j \, dx \right) c_j^{n+1} &= \sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} (\psi_i \psi_j - \Delta t \alpha \nabla \psi_i \cdot \nabla \psi_j) \, dx \right) c_j^n - \\ &\int_{\Omega} (u_0(\mathbf{x}, t_{n+1}) - u_0(\mathbf{x}, t_n) + \Delta t \alpha \nabla u_0(\mathbf{x}, t_n) \cdot \nabla \psi_i) \, dx \\ &+ \Delta t \int_{\Omega} f \psi_i \, dx - \Delta t \int_{\partial\Omega_N} g \psi_i \, ds, \quad i \in \mathcal{I}_s \end{aligned}$$

Finite element basis functions

- $B(\mathbf{x}, t_n) = \sum_{j \in \mathcal{I}_b} U_j^n \varphi_j$
- $\psi_i = \varphi_{\nu(j)}$, $j \in \mathcal{I}_s$
- $\nu(j)$, $j \in \mathcal{I}_s$, are the node numbers corresponding to all nodes without a Dirichlet condition

$$\begin{aligned} u^n &= \sum_{j \in \mathcal{I}_b} U_j^n \varphi_j + \sum_{j \in \mathcal{I}_s} c_{1,j} \varphi_{\nu(j)}, \\ u^{n+1} &= \sum_{j \in \mathcal{I}_b} U_j^{n+1} \varphi_j + \sum_{j \in \mathcal{I}_s} c_j \varphi_{\nu(j)} \end{aligned}$$

$$\begin{aligned} \sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} \varphi_i \varphi_j \, dx \right) c_j &= \sum_{j \in \mathcal{I}_s} \left(\int_{\Omega} (\varphi_i \varphi_j - \Delta t \alpha \nabla \varphi_i \cdot \nabla \varphi_j) \, dx \right) c_{1,j} - \\ &\sum_{j \in \mathcal{I}_b} \int_{\Omega} \left(\varphi_i \varphi_j (U_j^{n+1} - U_j^n) + \Delta t \alpha \nabla \varphi_i \cdot \nabla \varphi_j U_j^n \right) \, dx \\ &+ \Delta t \int_{\Omega} f \varphi_i \, dx - \Delta t \int_{\partial\Omega_N} g \varphi_i \, ds, \quad i \in \mathcal{I}_s \end{aligned}$$

Modification of the linear system; the raw system

- Drop boundary function
- Compute as if there are not Dirichlet conditions
- Modify the linear system to incorporate Dirichlet conditions
- \mathcal{I}_s holds the indices of all nodes $\{0, 1, \dots, N = N_n - 1\}$

$$\begin{aligned} \sum_{j \in \mathcal{I}_s} \underbrace{\left(\int_{\Omega} \varphi_i \varphi_j \, dx \right)}_{M_{i,j}} c_j &= \sum_{j \in \mathcal{I}_s} \underbrace{\left(\int_{\Omega} \varphi_i \varphi_j \, dx \right)}_{M_{i,j}} - \Delta t \underbrace{\int_{\Omega} \alpha \nabla \varphi_i \cdot \nabla \varphi_j \, dx}_{K_{i,j}} c_{1,j} \\ &+ \Delta t \underbrace{\int_{\Omega} f \varphi_i \, dx - \Delta t \int_{\partial\Omega_N} g \varphi_i \, ds}_{f_i}, \quad i \in \mathcal{I}_s \end{aligned}$$

Modification of the linear system; setting Dirichlet conditions

$$Mc = b, \quad b = Mc_1 - \Delta t K c_1 + \Delta t f$$

For each k where a Dirichlet condition applies, $u(x_k, t_{n+1}) = U_k^{n+1}$,

- set row k in M to zero and 1 on the diagonal: $M_{k,j} = 0$, $j \in \mathcal{I}_s$, $M_{k,k} = 1$
- $b_k = U_k^{n+1}$

Or apply the slightly more complicated modification which preserves symmetry of M

Modification of the linear system; Backward Euler example

Backward Euler discretization in time gives a more complicated coefficient matrix:

$$Ac = b, \quad A = M + \Delta t K, \quad b = Mc_1 + \Delta t f$$

- Set row k to zero and 1 on the diagonal: $M_{k,j} = 0$, $j \in \mathcal{I}_s$, $M_{k,k} = 1$
- Set row k to zero: $K_{k,j} = 0$, $j \in \mathcal{I}_s$
- $b_k = U_k^{n+1}$

Observe: $A_{k,k} = M_{k,k} + \Delta t K_{k,k} = 1 + 0$, so $c_k = U_k^{n+1}$

Analysis of the discrete equations

The diffusion equation $u_t = \alpha u_{xx}$ allows a (Fourier) wave component

$$u = A_e^n e^{ikx}, \quad A_e = e^{-\alpha k^2 \Delta t}$$

Numerical schemes often allow the similar solution

$$U_q^n = A^n e^{ikx}$$

- A : amplification factor to be computed
- How good is this A compared to the exact one?

Handy formulas

$$\begin{aligned} [D_t^+ A^n e^{ikq\Delta x}]^n &= A^n e^{ikq\Delta x} \frac{A - 1}{\Delta t}, \\ [D_t^- A^n e^{ikq\Delta x}]^n &= A^n e^{ikq\Delta x} \frac{1 - A^{-1}}{\Delta t}, \\ [D_t A^n e^{ikq\Delta x}]^{n+\frac{1}{2}} &= A^{n+\frac{1}{2}} e^{ikq\Delta x} \frac{A^{\frac{1}{2}} - A^{-\frac{1}{2}}}{\Delta t} = A^n e^{ikq\Delta x} \frac{A - 1}{\Delta t}, \\ [D_x D_x A^n e^{ikq\Delta x}]_q &= -A^n \frac{4}{\Delta x^2} \sin^2 \left(\frac{k\Delta x}{2} \right) \end{aligned}$$

Amplification factor for the Forward Euler method; results

Introduce $p = k\Delta x/2$ and $C = \alpha\Delta t/\Delta x^2$:

$$A = 1 - 4C \underbrace{\frac{\sin^2 p}{1 - \frac{2}{3}\sin^2 p}}_{\text{from } M}$$

(See notes for details)

Stability: $|A| \leq 1$:

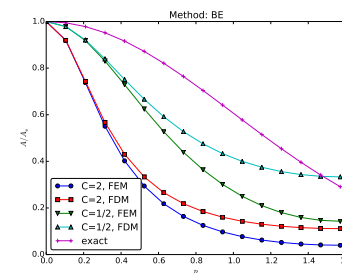
$$C \leq \frac{1}{6} \Rightarrow \Delta t \leq \frac{\Delta x^2}{6\alpha}$$

Finite differences: $C \leq \frac{1}{2}$, so finite elements give a *stricter* stability criterion for this PDE!

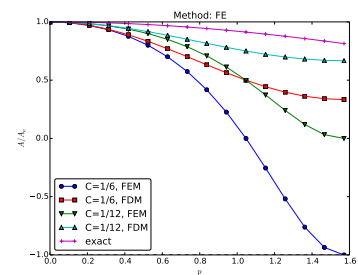
Amplification factor for the Backward Euler method; results

Coarse meshes:

$$A = \left(1 + 4C \frac{\sin^2 p}{1 + \frac{2}{3}\sin^2 p} \right)^{-1} \quad (\text{unconditionally stable})$$



Amplification factors for smaller time steps; Forward Euler



Amplification factors for smaller time steps; Backward Euler

